Magnetic properties of periodic nonuniform spin-$\frac{1}{2}$ XX chains in a random Lorentzian transverse field

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Abstract

Using continued fractions we examine the density of states, transverse magnetization and static transverse linear susceptibility of a few periodic nonuniform spin-$\frac{1}{2}$ XX chains in a random Lorentzian transverse field.

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The one-dimensional spin-$\frac{1}{2}$ XY model was introduced in 1961 by Lieb, Schultz and Mattis.[1] The authors of that celebrated paper found that several statistical mechanics calculations for that spin model could be performed exactly because it can be rewritten as a model of non-interacting spinless fermions with the help of the Jordan-Wigner transformation. Evidently, the formulation of the spin-$\frac{1}{2}$ XY chain in terms of fermions permits one to give a magnetic interpretation to the results derived for one-dimensional tight-binding spinless fermions. As an example of where this relationship has been exploited one can cite the papers on the Lloyd model[2,3] and corresponding papers on the spin-$\frac{1}{2}$ XX chain in a random Lorentzian transverse field.[4,5] The work reported in the present paper has been inspired by some results on one-dimensional tight-binding Hamiltonians for periodically modulated lattices[6,7] and spinless Falicov-Kimball model.[8,9] Combining the approach developed in those papers and the treatment of the Lloyd model presented in Refs. 2, 3 we shall calculate exactly the random-averaged one-fermion Green functions (that yield the density of states and therefore the thermodynamics) for the periodic nonuniform spin-$\frac{1}{2}$ XX chain in a random Lorentzian transverse field. We shall treat a few particular chains in order to discuss the changes in the density of states and magnetic properties induced by periodic nonuniformity and diagonal disorder. It should be noted, in passing, that the periodic nonuniform spin-$\frac{1}{2}$ XX chain was considered in several papers dealing with the spin-Peierls instability in a spin-$\frac{1}{2}$ XX chain[10,11] (see also Refs. 12-16). However, those papers concentrated on the influence of the structural degrees of freedom upon the magnetic ones, rather than on the properties of a magnetic chain with regularly alternating exchange couplings. One should also mention a study of a spin-$\frac{1}{2}$ XX model on a one-dimensional superlattice[17] (such a model can be viewed as a nonuniform chain with periodically varying exchange coupling) but consideration was restricted to the excitation spectrum. Our communication is also related to the work in Ref. 18 and may be viewed as a further study of the effects of periodic nonuniformity and randomness on magnetic properties of spin-$\frac{1}{2}$ chains.

Let us consider a cyclic nonuniform XX chain of $N \to \infty$ spins $\frac{1}{2}$ in a transverse field described by the Hamiltonian

$$H = \sum_{n=1}^{N} \Omega_n s_n^z + 2\sum_{n=1}^{N} I_n \left(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y \right)$$
$$= \sum_{n=1}^{N} \Omega_n \left(s_n^+ s_n^- - \frac{1}{2} \right) + \sum_{n=1}^{N} I_n \left(s_n^+ s_{n+1}^- + s_n^- s_{n+1}^+ \right). \qquad (1)$$

Here Ω_n is the transverse field at the site n, and is assumed to be a random variable with the

Lorentzian probability distribution

$$p(\Omega_n) = \frac{1}{\pi}\frac{\Gamma_n}{(\Omega_n - \Omega_{0n})^2 + \Gamma_n^2}, \tag{2}$$

Ω_{0n} is the mean value of the transverse field at the site n, and Γ_n is the width of its distribution. $2I_n$ is the exchange coupling between the sites n and $n+1$. After making use of the Jordan-Wigner transformation the model is recasted into a chain of spinless fermions governed by the Hamiltonian

$$H = \sum_{n=1}^{N} \Omega_n \left(c_n^+ c_n - \frac{1}{2}\right) + \sum_{n=1}^{N} I_n \left(c_n^+ c_{n+1} - c_n c_{n+1}^+\right) \tag{3}$$

(the boundary term that is non-essential for the calculation of thermodynamic quantities has been omitted). Note, that for the non-random case ($\Gamma_n = 0$) assuming the transverse field in (3) to be uniform one arises at the Hamiltonian considered in Ref. 6. In addition, after substitution $\Omega_n \to U w_n$, $I_n \to -t$, Eq. (3) transforms into the Hamiltonian of a one-dimensional spinless Falicov-Kimball model in the notations used in Refs. 8, 9. In model (3), considered here, not only the transverse fields that are independent random Lorentzian variables having the mean values and widths of their distribution, but also the exchange couplings between neighbouring spins, vary from site to site.

Let us introduce the temperature double-time Green functions $G_{nm}^{\mp}(t) = \mp\mathrm{i}\theta(\pm t)\langle\{c_n(t), c_m^+(0)\}\rangle$, $G_{nm}^{\mp}(t) = (1/2\pi)\int_{-\infty}^{\infty} \mathrm{d}\omega \exp\left(-\mathrm{i}\omega t\right) G_{nm}^{\mp}(\omega \pm \mathrm{i}\epsilon)$, $\epsilon \to +0$, where the angular brackets denote the thermodynamic average. Utilising a set of equations for $G_{nm}^{\mp} \equiv G_{nm}^{\mp}(\omega \pm \mathrm{i}\epsilon)$, and performing random averaging using contour integrals[2–5], one finds the following set of equations for the random-averaged Green functions

$$(\omega \pm \mathrm{i}\Gamma_n - \Omega_{0n})\,\overline{G_{nm}^{\mp}} - I_{n-1}\overline{G_{n-1,m}^{\mp}} - I_n\overline{G_{n+1,m}^{\mp}} = \delta_{nm}. \tag{4}$$

Here $\overline{(\ldots)} \equiv \int_{-\infty}^{\infty}\mathrm{d}\Omega_1 p(\Omega_1)\ldots\int_{-\infty}^{\infty}\mathrm{d}\Omega_N p(\Omega_N)(\ldots)$. Our task is to evaluate the diagonal random-averaged Green functions $\overline{G_{nn}^{\mp}}$, the imaginary parts of which give the random-averaged density of states $\overline{\rho(\omega)}$,

$$\overline{\rho(\omega)} = \mp\frac{1}{\pi N}\sum_{n=1}^{N}\mathrm{Im}\overline{G_{nn}^{\mp}} \tag{5}$$

that in its turn, yields thermodynamic properties of spin model (1). It is a simple matter to obtain from Eq. (4) the following representation for $\overline{G_{nn}^{\mp}}$

$$\overline{G_{nn}^{\mp}} = \frac{1}{\omega \pm \mathrm{i}\Gamma_n - \Omega_{0n} - \Delta_n^- - \Delta_n^+},$$

$$\Delta_n^- = \cfrac{I_{n-1}^2}{\omega \pm \mathrm{i}\Gamma_{n-1} - \Omega_{0,n-1} - \cfrac{I_{n-2}^2}{\omega\pm\mathrm{i}\Gamma_{n-2}-\Omega_{0,n-2}- \ddots}},$$

$$\Delta_n^+ = \cfrac{I_{n}^2}{\omega \pm \mathrm{i}\Gamma_{n+1} - \Omega_{0,n+1} - \cfrac{I_{n+1}^2}{\omega\pm\mathrm{i}\Gamma_{n+2}-\Omega_{0,n+2}- \ddots}}. \qquad (6)$$

Eqs. (5), (6) are extremely useful for examining thermodynamic properties of periodic nonuniform spin-$\frac{1}{2}$ XX chain in a random Lorentzian transverse field when periodic continued fractions emerge.

Consider at first, a non-random case. For a regular alternating chain $\Omega_1 I_1 \Omega_2 I_2 \Omega_3 I_3 \Omega_1 I_1 \Omega_2 I_2 \Omega_3 I_3 \ldots$ one generates periodic continued fractions having a period 3, and after some calculations one gets

$$\rho(\omega) = \begin{cases} 0, & \text{if} \quad \omega < c_6, \quad c_5 < \omega < c_4, \quad c_3 < \omega < c_2, \quad c_1 < \omega, \\ \frac{1}{3\pi}\frac{\vert\mathcal{X}(\omega)\vert}{\sqrt{\mathcal{C}(\omega)}}, & \text{if} \quad c_6 < \omega < c_5, \quad c_4 < \omega < c_3, \quad c_2 < \omega < c_1; \end{cases}$$

$$\mathcal{X}(\omega) = I_1^2 + I_2^2 + I_3^2 - (\omega - \Omega_1)(\omega - \Omega_2) - (\omega - \Omega_1)(\omega - \Omega_3) - (\omega - \Omega_2)(\omega - \Omega_3),$$

$$\mathcal{C}(\omega) = 4I_1^2 I_2^2 I_3^2 - \left[I_1^2(\omega - \Omega_3) + I_2^2(\omega - \Omega_1) + I_3^2(\omega - \Omega_2) - (\omega - \Omega_1)(\omega - \Omega_2)(\omega - \Omega_3)\right]^2 = -\prod_{j=1}^{6}(\omega - c_j). \qquad (7)$$

Here $c_1 \geq \ldots \geq c_6$ denote six roots of the equation $\mathcal{C}(\omega) = 0$ that can be found by solving two cubic equations. For a regular alternating chain $\Omega_1 I_1 \Omega_2 I_2 \Omega_3 I_3 \Omega_4 I_4 \Omega_1 I_1 \Omega_2 I_2 \Omega_3 I_3 \Omega_4 I_4 \ldots$ periodic continued fractions having period 4 emerge, and after some calculations one finds

$$\rho(\omega) = \begin{cases} 0, & \text{if} \quad \omega < d_8, \quad d_7 < \omega < d_6, \quad d_5 < \omega < d_4, \quad d_3 < \omega < d_2, \quad d_1 < \omega, \\ \frac{1}{4\pi}\frac{\vert\mathcal{W}(\omega)\vert}{\sqrt{\mathcal{D}(\omega)}}, & \text{if} \quad d_8 < \omega < d_7, \quad d_6 < \omega < d_5, \quad d_4 < \omega < d_3, \quad d_2 < \omega < d_1; \end{cases}$$

$$\begin{aligned} \mathcal{W}(\omega) = {} & I_1^2(2\omega - \Omega_3 - \Omega_4) + I_2^2(2\omega - \Omega_1 - \Omega_4) + I_3^2(2\omega - \Omega_1 - \Omega_2) + I_4^2(2\omega - \Omega_2 - \Omega_3) \\ & -(\omega - \Omega_1)(\omega - \Omega_2)(\omega - \Omega_3) - (\omega - \Omega_1)(\omega - \Omega_2)(\omega - \Omega_4) \\ & -(\omega - \Omega_1)(\omega - \Omega_3)(\omega - \Omega_4) - (\omega - \Omega_2)(\omega - \Omega_3)(\omega - \Omega_4), \\ \mathcal{D}(\omega) = {} & 4I_1^2 I_2^2 I_3^2 I_4^2 - [(\omega - \Omega_1)(\omega - \Omega_2)(\omega - \Omega_3)(\omega - \Omega_4) \\ & -I_1^2(\omega - \Omega_3)(\omega - \Omega_4) - I_2^2(\omega - \Omega_1)(\omega - \Omega_4) \\ & -I_3^2(\omega - \Omega_1)(\omega - \Omega_2) - I_4^2(\omega - \Omega_2)(\omega - \Omega_3) \\ & +I_1^2 I_3^2 + I_2^2 I_4^2\big]^2 = -\prod_{j=1}^{8}(\omega - d_j). \end{aligned} \qquad (8)$$

Here, $d_1 \geq \ldots \geq d_8$ are the eight roots of the equation $\mathcal{D}(\omega) = 0$ that can be found by solving two equations of 4th order. Let us note that all c_j and d_j are real since they can be viewed as eigenvalues of symmetric matrices.[6]

The simplest periodic nonuniform spin-$\frac{1}{2}$ XX chain in a random Lorentzian transverse field $\Omega_{01}\Gamma_1 I_1 \Omega_{02}\Gamma_2 I_2 \Omega_{01}\Gamma_1 I_1 \Omega_{02}\Gamma_2 I_2 \ldots$ requires a calculation of periodic continued fractions with period 2. The random-averaged density of states for this case becomes

$$\overline{\rho(\omega)} = \frac{1}{2\pi} \frac{\mid \mathcal{Y}(\omega) \mid}{\mathcal{B}(\omega)};$$

$$\mathcal{Y}(\omega) = (\Gamma_1 + \Gamma_2)\sqrt{\frac{\mathcal{B}(\omega) + \mathcal{B}'(\omega)}{2}} - \operatorname{sgn}\mathcal{B}''(\omega)\ (2\omega - \Omega_{01} - \Omega_{02})\sqrt{\frac{\mathcal{B}(\omega) - \mathcal{B}'(\omega)}{2}},$$

$$\mathcal{B}(\omega) = \sqrt{\left(\mathcal{B}'(\omega)\right)^2 + \left(\mathcal{B}''(\omega)\right)^2},$$

$$\mathcal{B}'(\omega) = \left[(\omega - \Omega_{01})(\omega - \Omega_{02}) - \Gamma_1\Gamma_2 - I_1^2 - I_2^2\right]^2 - \left[(\omega - \Omega_{01})\Gamma_2 + (\omega - \Omega_{02})\Gamma_1\right]^2 - 4I_1^2 I_2^2,$$

$$\mathcal{B}''(\omega) = 2\left[(\omega - \Omega_{01})(\omega - \Omega_{02}) - \Gamma_1\Gamma_2 - I_1^2 - I_2^2\right]\left[(\omega - \Omega_{01})\Gamma_2 + (\omega - \Omega_{02})\Gamma_1\right]. \quad (9)$$

In principal, there are no difficulties in considering more complicated periodic nonuniform chains apart from the fact that the calculations become somewhat cumbersome.

Let us turn to a discussion of the results obtained for the density of states. First, note that in the limit of a uniform transverse field and exchange coupling, Eqs. (7) and (8) reproduce the well-known result for the uniform spin-$\frac{1}{2}$ XX chain in a transverse field: $\rho(\omega) = 1/\pi\sqrt{4I^2 - (\omega - \Omega)^2}$ if $4I^2 - (\omega - \Omega)^2 > 0$ and $\rho(\omega) = 0$, otherwise. This result for the uniform chain also follows from (9) if $\Omega_{01} = \Omega_{02} = \Omega$, $\Gamma_1 = \Gamma_2 = 0$, $I_1 = I_2 = I$. The density of states (9) contains the result for uniform spin-$\frac{1}{2}$ XX chain in a random Lorentzian transverse field[4] $\overline{\rho(\omega)} = \mp(1/\pi)\mathrm{Im}\left[1/\sqrt{(\omega \pm \mathrm{i}\Gamma - \Omega_0)^2 - 4I^2}\right]$ if $\Omega_{01} = \Omega_{02} = \Omega_0$, $\Gamma_1 = \Gamma_2 = \Gamma$, $I_1 = I_2 = I$. In addition, the density of states (9), in the non-random limit $\Gamma_1 = \Gamma_2 = 0$, coincides with the density of states (8) with $\Omega_1 = \Omega_3$, $\Omega_2 = \Omega_4$, $I_1 = I_3$, $I_2 = I_4$, i.e. for a regular alternarting chain $\Omega_1 I_1 \Omega_2 I_2 \Omega_1 I_1 \Omega_2 I_2 \ldots$ as should be expected.

In Figs. 1 - 3 we display the density of states, together with both the dependencies of the transverse magnetization

$$\overline{m_z} = -\frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}E\overline{\rho(E)}\tanh\frac{E}{2kT} \quad (10)$$

on the transverse field at zero temperature, and the static transverse linear susceptibility

$$\overline{\chi_{zz}} = -\frac{1}{kT}\int_{-\infty}^{\infty} \mathrm{d}E\overline{\rho(E)}\frac{1}{4\cosh^2\frac{E}{2kT}} \quad (11)$$

on temperature, for few particular chains considered. Initially, let us discuss a non-random case. The main result of introducing the nonuniformity is a splitting of the initial magnon

band with the edges $\Omega - 2 \mid I \mid$, $\Omega + 2 \mid I \mid$ into several subbands. The edges of the subbands are determined by the roots of equations $\mathcal{C}(\omega) = 0$, $\mathcal{D}(\omega) = 0$. $\rho(\omega)$ is positive inside the subbands, tends to infinity inversely proportionally to the square root of ω when ω approaches the subbands edges, and is equal to zero outside the subbands. For special values of parameters, the roots of the equations that determine the subbands edges may become multiple, the zeros in denominator and numerator in the expression for the density of states cancel each other, and as a result one observes a smaller number of subbands. In Figs. 1a, 2a we show $\rho(\omega)$ for some periodic nonuniform chains having periods 3 and 4 to demonstrate the energy band scheme in the presence of nonuniformity. Note that the splitting caused by periodic nonuniformity is not surprising, since the periodic nonuniform chain can be viewed as a uniform chain with a crystalline unit cell containing several sites of the initial lattice. On the other hand, one expects several subbands for a crystal having several atoms per unit cell (see for example Ref. 19). We now turn to the density of states given by (9). First, note that in the non-random case one finds two magnon subbands the edges of which are given by

$$\{b_1, b_2, b_3, b_4\} = \left\{ \frac{1}{2} \left[\Omega_1 + \Omega_2 \pm \sqrt{(\Omega_1 - \Omega_2)^2 + 4 \left(\mid I_1 \mid \pm \mid I_2 \mid \right)^2} \right] \right\} \tag{12}$$

(Fig. 3a). Introduction of the uniform diagonal Lorentzian disorder $\Gamma_1 = \Gamma_2 = \Gamma$ results in smearing out of the edges of subbands (Fig. 3b). For extremely nonuniform diagonal Lorentzian disorder $\Gamma_1 = 0$, $\Gamma_2 \neq 0$ and with a small strength of disorder only one subband may be mainly smoothed, but with increasing of the strength of disorder both subbands become smeared out (Fig. 3c).

The described dependencies of the density of magnon states on introduction of periodic nonuniformity and disorder affects the behaviour of thermodynamic quantities of the spin model. For example, the temperature dependence of the specific heat $\overline{c} = \int_{-\infty}^{\infty} \mathrm{d}E \overline{\rho(E)} \left(\frac{E}{2kT} \right)^2 / \cosh^2 \frac{E}{2kT}$ for a non-random periodic chain may exhibit a two-peak structure consisting of low-temperature and high-temperature peaks. Let us comment in some detail on the magnetic properties of the spin chains considered. The splitting of the magnon band into subbands caused by nonuniformity has interesting consequences for those properties. Consider for example the transverse magnetization (10). Since for $T \to 0$, $\tanh \frac{E}{2kT}$ tends either to -1 if $E < 0$, or to 1 if $E > 0$, one immediately finds because of the appearance of subbands that the low-temperature dependence of m_z against Ω in the non-random case must be composed of sharply increasing parts (when, with increasing Ω, $E = 0$ moves inside each subband from its top to its bottom) separated by horizontal parts (when, with increasing of Ω, $E = 0$ moves inside the gaps). Evidently a number of plateaus in the low-temperature dependence of

the transverse magnetization on transverse field is determined by a number of subbands. Every cusp in the the dependence of the transverse magnetization on Ω induces a singularity in the dependence of the static transverse linear susceptibility (11) on Ω. One can easily show that the dependence $\overline{\chi_{zz}}$ against Ω, at $T=0$, is the same as the dependence of $\overline{\rho(\omega)}$ against $\Omega-\omega$. The latter dependence can be derived from the densities of states depicted in Figs. 1-3. The value of $\overline{\chi_{zz}}$ at $T=0$ in the temperature dependence of $\overline{\chi_{zz}}$ at $\Omega=0$ is determined by the value of $\overline{\rho(0)}$. Therefore, the nonuniformity and randomness may essentially effect this value as well as the temperature dependence of the static transverse linear susceptibility. In different temperature regions one finds both an enhancement (and even a divergence, as in Fig. 3g), or suppressing of the curves $-\overline{\chi_{zz}}$ versus T. This can be seen nicely in Figs. 1c, 2c, 3g, 3h, 3i.

To summarize, using continued fractions we have obtained rigorously the density of magnon states for periodic nonuniform spin-$\frac{1}{2}$ XX chain in a random Lorentzian transverse field. Continued fraction representation of the solution of Eq. (4) is extremely useful for calculation of the density of magnon states. The attractive features of this approach can be seen even for the uniform case. In this case one omits performing twice the Fourier transformation while solving Eq. (4) in a standard manner and evaluates straightforwardly the desired $\overline{\rho(\omega)}$. The advantages of the continued fraction approach become clear while treating periodic chains already with the smallest period of 2. Periodic nonuniformity leads to a splitting of the magnon band into subbands that in its turn leads to the appearance of new cusps and singularities in the low-temperature dependences of the transverse magnetization and the static transverse linear susceptibility on transverse field, respectively. In the random case the spectacular changes in these dependences are smoothed. Periodic nonuniformity and randomness may either enhance or suppress the temperature dependence of $-\overline{\chi_{zz}}$. Changing the degree of periodic nonuniformity one may to some extent influence the detailed shapes $\overline{m_z}$ or $\overline{\chi_{zz}}$ against Ω, or $\overline{\chi_{zz}}$ against T. The described approach may be of considerable use for examining simple models of spin-Peierls instabilities, especially in the presence of disorder. Analysis of the thermodynamic properties of non-random and random Lorentzian periodic nonuniform spin-$\frac{1}{2}$ XX chain in a transverse field and its stability with respect to a lattice distorsion will be given in a separate paper.

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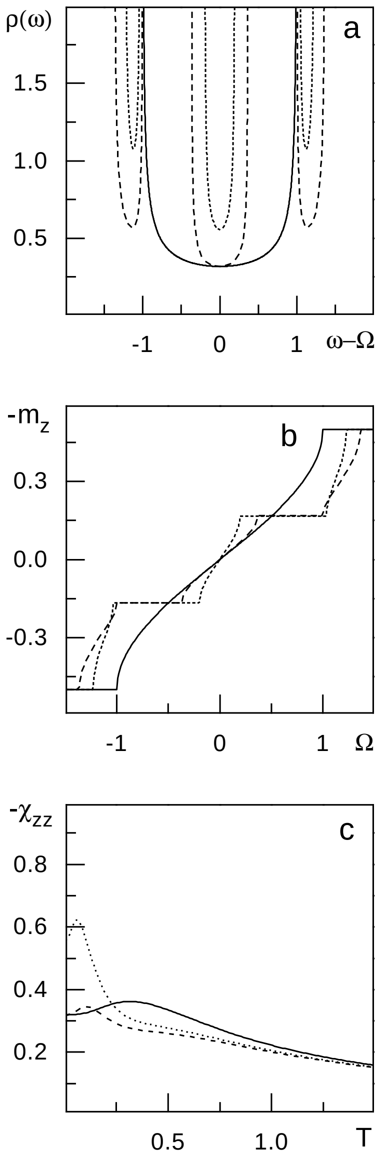

Figure 1:

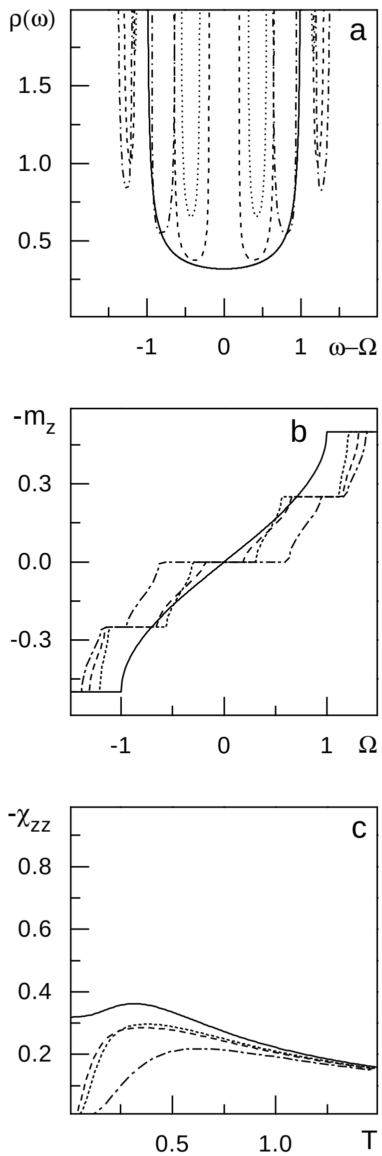

Figure 2:

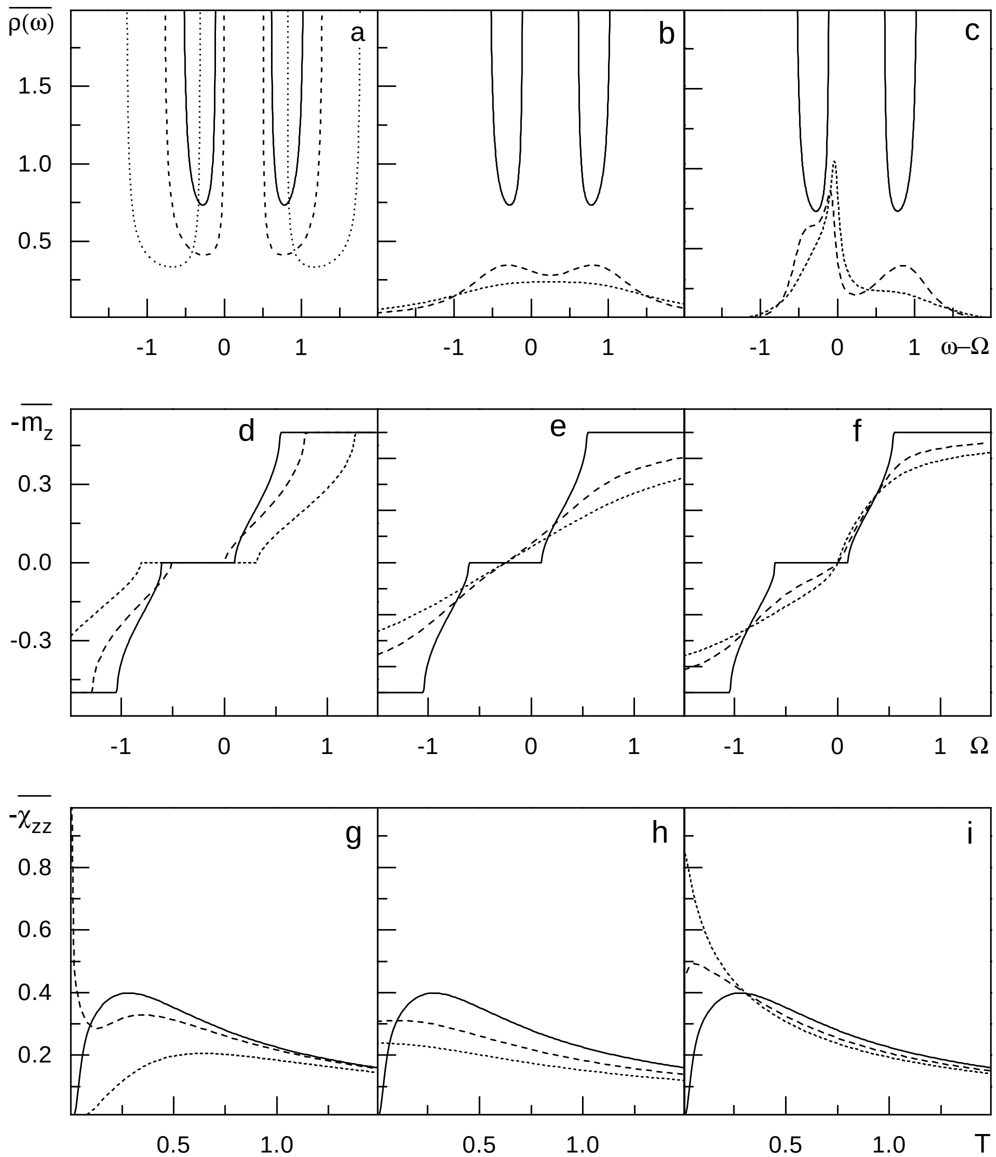

Figure 3:

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FIG. 1. Density of states (a), transverse magnetization versus transverse field Ω at $T = 0$ (b), and static transverse linear susceptibility versus temperature at $\Omega = 0$ (c), for the nonuniform chain $\Omega I_1 \Omega I_2 \Omega I_3 \Omega I_1 \Omega I_2 \Omega I_3 \ldots$, $I_1 = 0.5$. $I_2 = 0.5$, $I_3 = 0.5$ (solid lines); $I_2 = 0.5$, $I_3 = 1$ (dashed lines); $I_2 = 0.25$, $I_3 = 1$ (dotted lines).

FIG. 2. The same as in Fig. 1 for the nonuniform chain $\Omega I_1 \Omega I_2 \Omega I_3 \Omega I_4 \Omega I_1 \Omega I_2 \Omega I_3 \Omega I_4 \ldots$, $I_1 = 0.5$. $I_2 = 0.5$, $I_3 = 0.5$, $I_4 = 0.5$ (solid lines); $I_2 = 0.5$, $I_3 = 0.5$, $I_4 = 1$ (dashed lines); $I_2 = 0.5$, $I_3 = 0.25$, $I_4 = 1$ (dotted lines); $I_2 = 1$, $I_3 = 0.25$, $I_4 = 1$ (dash-dotted lines).

FIG. 3. Density of states (a,b,c), transverse magnetization versus transverse field Ω at $T = 0$ (d,e,f), and static transverse linear susceptibility versus temperature at $\Omega = 0$ (g,h,i), for the nonuniform random chain $\Omega_{01}\Gamma_1 I_1 \Omega_{02}\Gamma_2 I_2 \Omega_{01}\Gamma_1 I_1 \Omega_{02}\Gamma_2 I_2 \ldots$, $I_1 = 0.5$, $\Omega_{01} = \Omega$, $\Omega_{01} = 0.5+\Omega$. a, d, g: non-random case $\Gamma_1 = \Gamma_2 = 0$, $I_2 = 0.25$ (solid lines), $I_2 = 0.5$ (dashed lines), $I_2 = 1$ (dotted lines); b, e, h: uniform disorder $I_2 = 0.25$, $\Gamma_1 = \Gamma_2 = 0$ (solid lines), $\Gamma_1 = \Gamma_2 = 0.5$ (dashed lines), $\Gamma_1 = \Gamma_2 = 1$ (dotted lines); c, f, i: nonuniform disorder $I_2 = 0.25$, $\Gamma_1 = 0$, $\Gamma_2 = 0$ (solid lines), $\Gamma_2 = 0.5$ (dashed lines), $\Gamma_2 = 1$ (dotted lines).